The interaction of water with environmentally relevant surfaces

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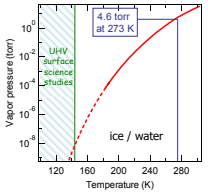
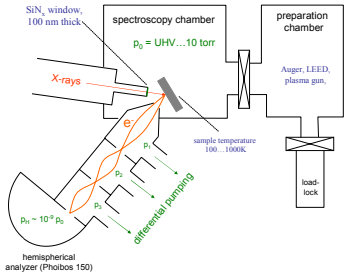
Introduction

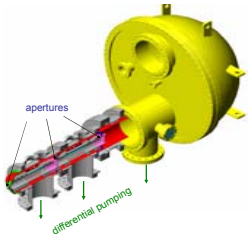
Probing the coverage and chemical speciation of molecules at surfaces are of fundamental interest in molecular environmental science. The concentration of water and its dissociation fragments at surfaces affect many highly important interfacial chemical processes and there exist no previous quantitative determinations of the coverage of water on clean metal surfaces at near ambient conditions. We have utilized Ambient Pressure Photoelectron Spectroscopy (AP-PES) to study the water/Cu(111) and Cu(110) systems at pressures up to 1 Torr in the temperature range 270-470 K.



Ambient-pressure PES at BL 11.0.2 at the Advanced Light Source

Main obstacle: scattering of electrons in the gas phase Solution: differentially pumped electrostatic lens (D.F. Ogletree et al., Rev. Sci. Instrum. 73 (2002) 3872.)

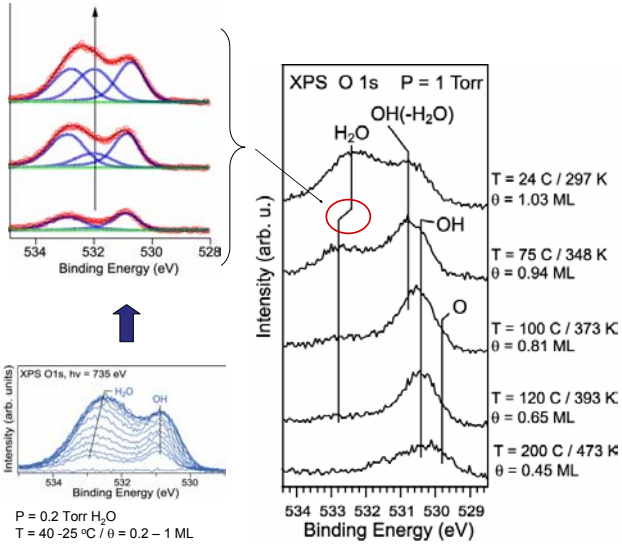




Conclusions

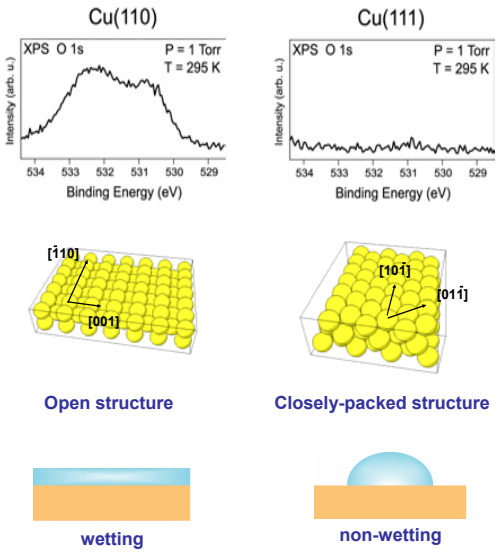
- **Surprisingly large difference in water chemistry on Cu(110) and Cu(111)**
  - **Cu(110)** 5 different species (H_2O, OH, and O in different local environments) were observed as a function of pressure and temperature.
  - **Cu(111)** No adsorbate species were observed.
- **OH-H_2O interaction is stronger than H_2O-H_2O interaction**
  H_2O molecules on hydroxylated metal surfaces are more strongly adsorbed than H_2O in pure water layer.
- **The wettability can be controlled by changing the adsorbed state of the preadsorbed O.**

Temperature dependence of surface speciation on Cu(110) at 1 torr

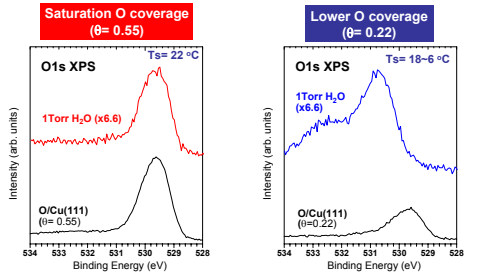


P = 0.2 Torr H_2O
T = 40 -25 °C / θ = 0.2 – 1 ML

Comparison of water adsorption on clean Cu(110) and Cu(111)



Control of wettability of Cu(111) by coadsorption of oxygen

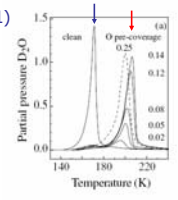


Discussion: mixed OH+H_2O phases on Pt(111)

Thermal Desorption Spectra C. Clay *et al.*, PRL 92 2004) 046102.

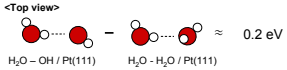
Clean Pt(111): **150-170 K;**

O-precovered Pt(111): 200 K
[OH+H_2O mixed phase]



DFT Calculation using pair potentials
G. S. Karlberg and G. Wahnström, J. Chem. Phys. 122 (2005) 194705.

<Top view>



Acknowledgement

This work was supported by the Office of Science, Biological and Environmental Research, Environmental Remediation Sciences Division, US Department of Energy. We would like to thank Ed Wong and Tolek Tyliszczak for their help.